



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 03:17 PM GMT

PDB ID : 4MJM
Title : Crystal Structure of the Inosine 5'-monophosphate Dehydrogenase, with a Short Internal Deletion of CBS Domain from Bacillus anthracis str. Ames
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-09-03
Resolution : 2.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

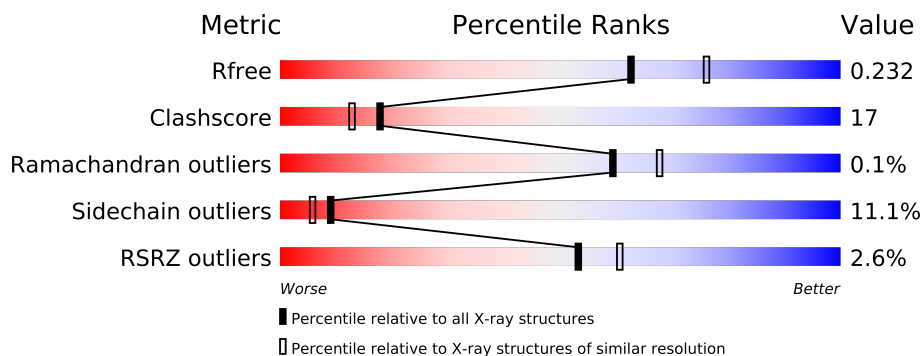
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	385	
1	B	385	
1	C	385	
1	D	385	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EDO	B	501	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10136 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inosine-5'-monophosphatedehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	1	0
			2411	1514	421	463	13			
1	B	328	Total	C	N	O	S	0	0	0
			2408	1514	419	461	14			
1	C	329	Total	C	N	O	S	0	0	0
			2412	1517	419	462	14			
1	D	328	Total	C	N	O	S	0	0	0
			2409	1514	422	460	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81W29
A	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
A	0	ALA	-	EXPRESSION TAG	UNP Q81W29
A	95	GLY	-	LINKER	UNP Q81W29
B	-2	SER	-	EXPRESSION TAG	UNP Q81W29
B	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
B	0	ALA	-	EXPRESSION TAG	UNP Q81W29
B	200	GLY	-	LINKER	UNP Q81W29
C	-2	SER	-	EXPRESSION TAG	UNP Q81W29
C	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
C	0	ALA	-	EXPRESSION TAG	UNP Q81W29
C	95	GLY	-	LINKER	UNP Q81W29
D	-2	SER	-	EXPRESSION TAG	UNP Q81W29
D	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
D	0	ALA	-	EXPRESSION TAG	UNP Q81W29
D	200	GLY	-	LINKER	UNP Q81W29

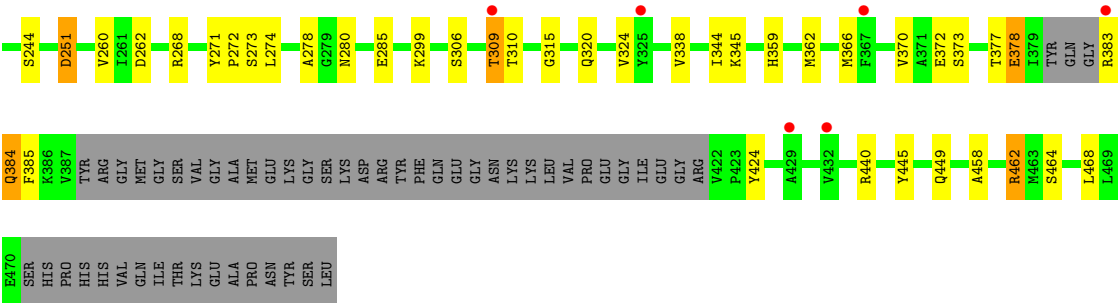
- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

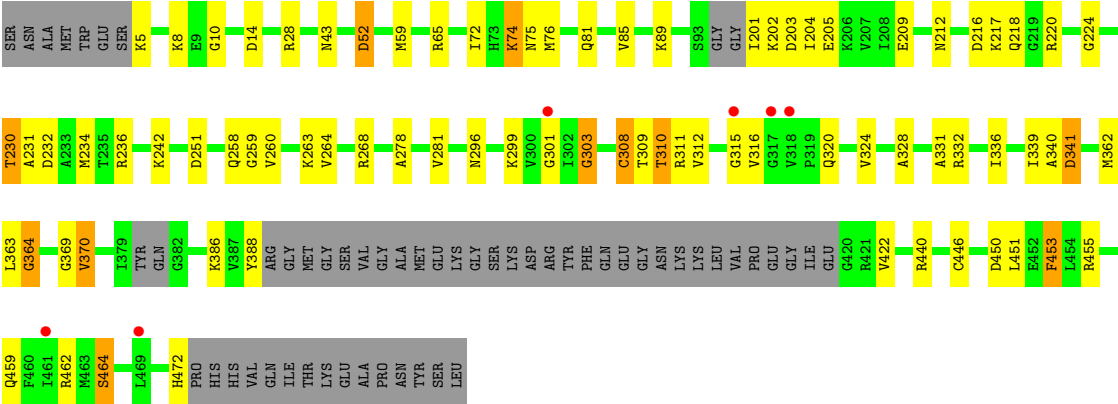
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	106	Total	O	0	0
			106	106		
3	C	108	Total	O	0	0
			108	108		
3	D	137	Total	O	0	0
			137	137		



● Molecule 1: Inosine-5'-monophosphatedehydrogenase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.33Å 84.25Å 84.31Å 110.01° 109.22° 109.19°	Depositor
Resolution (Å)	48.83 – 2.25 48.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.83-2.25) 94.0 (48.83-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.29 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.206 , 0.232 0.206 , 0.232	Depositor DCC
R_{free} test set	3948 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.1	EDS

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¹Intensities estimated from amplitudes.

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Property	Value	Source
Estimated twinning fraction	0.500 for -h-k-l,l,k 0.077 for -k,-l,h+k+l 0.077 for h+k+l,-h,-k 0.457 for -l,-h,h+k+l 0.457 for -k,h+k+l,-h 0.078 for h+k+l,-l,-h 0.078 for -l,h+k+l,-k 0.078 for -h-k-l,k,h 0.078 for l,k,-h-k-l 0.078 for l,h,k 0.078 for k,l,h 0.078 for k,-h-k-l,l 0.078 for -h-k-l,h,l 0.078 for h,-h-k-l,k 0.078 for h,l,-h-k-l 0.377 for l,-h-k-l,h 0.077 for -h,h+k+l,-l 0.458 for -h-k-l,l,k 0.377 for -h,-l,-k 0.377 for k,h,-h-k-l 0.078 for -h,-k,h+k+l 0.077 for -l,-k,-h 0.377 for h+k+l,-k,-l 0.079 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h-k-l,l,k	Depositor
L-test for twinning	$< L > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 79280 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10136	wwPDB-VP
Average B, all atoms (\AA^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	1/2438 (0.0%)	0.46	1/3290 (0.0%)
1	B	0.26	1/2436 (0.0%)	0.47	1/3287 (0.0%)
1	C	0.26	1/2440 (0.0%)	0.46	1/3294 (0.0%)
1	D	0.27	0/2436	0.46	1/3286 (0.0%)
All	All	0.27	3/9750 (0.0%)	0.46	4/13157 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	PRO	N-CD	5.31	1.55	1.47
1	C	272	PRO	N-CD	5.29	1.55	1.47
1	B	272	PRO	N-CD	5.13	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	303	GLY	C-N-CD	5.99	140.99	128.40
1	B	271	TYR	C-N-CD	5.75	140.47	128.40
1	C	271	TYR	C-N-CD	5.51	139.97	128.40
1	A	210	PHE	C-N-CD	5.38	139.71	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	THR	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2411	0	0	53	0
1	B	2408	0	0	44	0
1	C	2412	0	0	34	0
1	D	2409	0	0	47	0
2	A	12	0	18	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	12	0	18	0	0
3	A	113	0	0	12	0
3	B	106	0	0	12	0
3	C	108	0	0	11	0
3	D	137	0	0	12	0
All	All	10136	0	48	167	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (167) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:446:CYS:SG	3:D:616:HOH:O	2.25	0.93
1:A:205:GLU:O	1:A:209:GLU:N	2.21	0.73
1:A:230:THR:O	1:A:263:LYS:NZ	2.22	0.73
1:B:5:LYS:NZ	3:B:633:HOH:O	2.22	0.72
1:A:24:ASP:OD1	1:A:24:ASP:N	2.23	0.72
1:C:89:LYS:NZ	1:C:216:ASP:OD2	2.23	0.71
1:C:462:ARG:NH1	3:C:672:HOH:O	2.24	0.70
1:A:212:ASN:N	3:A:628:HOH:O	2.23	0.70
1:D:370:VAL:O	1:D:386:LYS:NZ	2.26	0.69
1:A:33:LYS:NZ	3:A:604:HOH:O	2.26	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:LYS:NZ	1:B:251:ASP:O	2.26	0.68
1:A:459:GLN:NE2	3:A:647:HOH:O	2.26	0.68
1:B:327:CYS:SG	3:B:647:HOH:O	2.51	0.68
1:A:94:GLY:N	1:A:203[B]:ASP:OD1	2.26	0.68
1:B:33:LYS:NZ	3:B:651:HOH:O	2.27	0.67
1:D:230:THR:OG1	1:D:231:ALA:N	2.28	0.67
1:B:300:VAL:O	1:B:341:ASP:N	2.28	0.66
1:A:366:MET:O	1:A:425:LYS:NZ	2.28	0.66
1:B:455:ARG:NH1	3:B:691:HOH:O	2.28	0.66
1:B:14:ASP:OD2	1:B:345:LYS:CE	2.44	0.66
1:D:43:ASN:ND2	1:D:212:ASN:O	2.30	0.65
1:B:87:LYS:NZ	3:B:678:HOH:O	2.28	0.65
1:D:472:HIS:NE2	3:D:697:HOH:O	2.30	0.65
1:B:310:THR:N	3:B:667:HOH:O	2.29	0.65
1:A:258:GLN:NE2	3:A:648:HOH:O	2.29	0.65
1:B:300:VAL:N	1:B:339:ILE:O	2.30	0.65
1:C:458:ALA:O	1:D:5:LYS:NZ	2.30	0.64
1:C:29:GLU:O	1:C:449:GLN:NE2	2.31	0.64
1:D:440:ARG:NH1	3:D:709:HOH:O	2.30	0.63
1:C:338:VAL:N	3:C:702:HOH:O	2.32	0.62
1:C:223:VAL:N	3:C:662:HOH:O	2.32	0.62
1:B:38:GLU:OE1	1:B:217:LYS:NZ	2.33	0.62
1:C:80:GLN:NE2	3:C:619:HOH:O	2.33	0.62
1:D:328:ALA:O	1:D:332:ARG:NE	2.32	0.62
1:A:74:LYS:NZ	1:A:251:ASP:OD1	2.32	0.62
1:D:230:THR:O	1:D:263:LYS:NZ	2.32	0.62
1:D:386:LYS:N	1:D:422:VAL:O	2.33	0.61
1:D:263:LYS:NZ	3:D:644:HOH:O	2.33	0.61
1:B:31:SER:N	1:B:449:GLN:O	2.33	0.61
1:C:280:ASN:ND2	3:C:637:HOH:O	2.32	0.61
1:D:369:GLY:N	3:D:635:HOH:O	2.32	0.61
1:C:232:ASP:N	1:C:232:ASP:OD1	2.33	0.60
1:A:305:GLY:O	1:D:472:HIS:ND1	2.35	0.60
1:D:308:CYS:SG	1:D:311:ARG:NH2	2.75	0.59
1:A:12:THR:OG1	1:A:15:ASP:OD1	2.20	0.59
1:C:31:SER:N	1:C:449:GLN:O	2.36	0.59
1:A:29:GLU:O	1:A:449:GLN:NE2	2.35	0.59
1:B:311:ARG:NH1	3:B:637:HOH:O	2.36	0.59
1:D:310:THR:O	1:D:315:GLY:N	2.36	0.59
1:C:66:GLN:NE2	3:C:635:HOH:O	2.37	0.58
1:A:352:LYS:NZ	3:A:642:HOH:O	2.36	0.58
1:D:331:ALA:O	1:D:336:ILE:N	2.37	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:278:ALA:O	1:D:299:LYS:N	2.37	0.57
1:A:8:LYS:O	1:D:462:ARG:N	2.38	0.57
1:C:27:PRO:O	1:C:440:ARG:NH1	2.38	0.57
1:B:298:VAL:O	1:B:339:ILE:N	2.37	0.57
1:C:220:ARG:NH1	1:C:244:SER:OG	2.39	0.56
1:B:43:ASN:ND2	3:B:635:HOH:O	2.38	0.56
1:C:93:SER:OG	1:C:221:LEU:N	2.39	0.56
1:A:303:GLY:N	3:A:669:HOH:O	2.39	0.56
1:D:281:VAL:O	1:D:301:GLY:N	2.39	0.56
1:C:310:THR:O	1:C:315:GLY:N	2.39	0.55
1:A:325:TYR:O	1:A:329:THR:OG1	2.24	0.55
1:D:234:MET:N	3:D:644:HOH:O	2.38	0.55
1:D:451:LEU:O	1:D:455:ARG:N	2.39	0.55
1:D:74:LYS:O	1:D:236:ARG:NH2	2.40	0.55
1:D:81:GLN:OE1	1:D:236:ARG:NH2	2.40	0.55
1:D:217:LYS:NZ	3:D:645:HOH:O	2.40	0.54
1:D:259:GLY:O	1:D:263:LYS:N	2.40	0.54
1:A:308:CYS:SG	1:A:309:THR:N	2.81	0.54
1:D:303:GLY:N	3:D:692:HOH:O	2.42	0.53
1:A:462:ARG:NH2	1:B:6:PHE:O	2.40	0.53
1:A:43:ASN:ND2	1:A:212:ASN:O	2.42	0.53
1:A:462:ARG:N	1:B:8:LYS:O	2.41	0.53
1:C:213:SER:N	3:C:674:HOH:O	2.42	0.53
1:B:52:ASP:OD1	1:B:52:ASP:N	2.42	0.52
1:A:34:THR:O	1:A:42:LEU:N	2.43	0.52
1:A:76:MET:O	1:A:236:ARG:NH2	2.42	0.52
1:A:93:SER:N	1:A:203[B]:ASP:OD1	2.42	0.52
1:B:74:LYS:NZ	1:B:251:ASP:OD2	2.43	0.52
1:B:75:ASN:ND2	3:B:610:HOH:O	2.43	0.52
1:D:450:ASP:OD2	1:D:453:PHE:N	2.43	0.51
1:A:225:ALA:N	1:A:247:ALA:O	2.43	0.51
1:A:300:VAL:O	1:A:341:ASP:N	2.43	0.51
1:D:205:GLU:O	1:D:209:GLU:N	2.43	0.51
1:A:22:LYS:NZ	3:A:636:HOH:O	2.43	0.51
1:C:78:ILE:O	1:C:82:ALA:N	2.44	0.51
1:C:462:ARG:N	1:D:8:LYS:O	2.44	0.51
1:C:440:ARG:NH2	3:C:641:HOH:O	2.42	0.50
1:C:372:GLU:OE2	1:C:372:GLU:N	2.44	0.50
1:A:364:GLY:N	3:A:682:HOH:O	2.44	0.50
1:C:204:ILE:O	1:C:208:ILE:N	2.44	0.50
1:D:364:GLY:N	3:D:678:HOH:O	2.44	0.50
1:D:296:ASN:OD1	1:D:296:ASN:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:28:ARG:NH1	3:D:636:HOH:O	2.44	0.50
1:B:30:VAL:O	1:B:440:ARG:NH1	2.45	0.50
1:A:93:SER:OG	1:A:203[B]:ASP:OD2	2.30	0.50
1:A:203[B]:ASP:N	1:A:203[B]:ASP:OD2	2.45	0.49
1:A:387:VAL:O	1:A:388:TYR:CB	2.60	0.49
1:A:464:SER:OG	1:B:15:ASP:OD2	2.30	0.48
1:A:88:VAL:O	1:A:91:SER:OG	2.31	0.48
1:A:206:LYS:O	1:A:210:PHE:N	2.46	0.48
1:A:39:SER:OG	3:A:673:HOH:O	2.20	0.48
1:C:278:ALA:O	1:C:299:LYS:N	2.47	0.48
1:A:218:GLN:NE2	3:A:605:HOH:O	2.46	0.48
1:D:216:ASP:OD1	1:D:220:ARG:N	2.47	0.48
1:C:86:ASP:OD2	1:C:90:ARG:NE	2.46	0.48
1:B:429:ALA:O	1:B:433:HIS:N	2.47	0.48
1:A:15:ASP:OD1	1:A:15:ASP:N	2.48	0.47
1:B:251:ASP:N	1:B:251:ASP:OD2	2.47	0.47
1:C:251:ASP:OD2	1:C:280:ASN:ND2	2.48	0.47
1:D:74:LYS:O	1:D:76:MET:N	2.47	0.47
1:B:280:ASN:OD1	1:B:299:LYS:NZ	2.48	0.47
1:C:370:VAL:O	1:C:373:SER:OG	2.33	0.47
1:D:52:ASP:OD1	1:D:75:ASN:ND2	2.47	0.47
1:A:227:VAL:N	1:A:249:VAL:O	2.47	0.46
1:B:358:ALA:O	1:B:455:ARG:NH1	2.49	0.46
1:B:380:TYR:CD2	1:B:380:TYR:C	2.89	0.46
1:A:235:THR:N	3:A:707:HOH:O	2.48	0.46
1:B:81:GLN:NE2	1:B:226:ALA:O	2.48	0.46
1:D:264:VAL:O	1:D:268:ARG:N	2.49	0.46
1:A:445:TYR:OH	1:B:253:ALA:O	2.33	0.46
1:B:37:SER:N	1:B:40:LEU:O	2.48	0.46
1:B:86:ASP:O	1:B:90:ARG:N	2.49	0.46
1:A:387:VAL:CG2	1:A:388:TYR:N	2.78	0.46
1:D:203:ASP:OD2	1:D:203:ASP:N	2.48	0.46
1:A:18:LEU:O	1:B:317:GLY:N	2.49	0.46
1:D:340:ALA:O	1:D:362:MET:N	2.48	0.46
1:C:378:GLU:O	1:C:384:GLN:NE2	2.48	0.46
1:B:220:ARG:NH1	3:B:611:HOH:O	2.49	0.45
1:C:244:SER:O	1:C:244:SER:OG	2.33	0.45
1:C:359:HIS:ND1	3:C:702:HOH:O	2.36	0.45
1:D:10:GLY:O	3:D:687:HOH:O	2.21	0.45
1:A:298:VAL:O	1:A:339:ILE:N	2.49	0.44
1:D:89:LYS:NZ	1:D:216:ASP:OD2	2.50	0.44
1:B:76:MET:O	1:B:236:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:52:ASP:OD2	1:D:52:ASP:N	2.49	0.44
1:D:72:ILE:N	1:D:224:GLY:O	2.51	0.44
1:B:443:MET:SD	3:B:616:HOH:O	2.61	0.44
1:C:320:GLN:O	1:C:324:VAL:N	2.50	0.43
1:A:213:SER:O	1:A:215:LYS:NZ	2.51	0.43
1:A:325:TYR:OH	1:B:2:TRP:O	2.36	0.43
1:B:79:GLU:O	1:B:83:GLU:N	2.52	0.43
1:D:320:GLN:O	1:D:324:VAL:N	2.52	0.43
1:A:15:ASP:OD2	1:D:464:SER:OG	2.36	0.43
1:A:300:VAL:N	1:A:339:ILE:O	2.52	0.42
1:A:232:ASP:OD2	3:A:616:HOH:O	2.22	0.42
1:B:325:TYR:O	1:B:329:THR:OG1	2.36	0.42
1:C:57:ALA:N	1:C:84:GLN:OE1	2.52	0.42
1:C:309:THR:N	3:C:649:HOH:O	2.52	0.42
1:B:23:SER:OG	1:B:25:VAL:O	2.36	0.42
1:B:270:LYS:CG	1:B:271:TYR:N	2.82	0.42
1:D:76:MET:O	1:D:236:ARG:NH2	2.52	0.42
1:C:309:THR:OG1	1:C:309:THR:O	2.35	0.42
1:C:464:SER:OG	3:C:663:HOH:O	2.22	0.42
1:B:380:TYR:O	1:B:380:TYR:CD2	2.73	0.41
1:D:204:ILE:N	3:D:601:HOH:O	2.53	0.41
1:A:36:LEU:N	1:A:40:LEU:O	2.54	0.41
1:C:268:ARG:NH1	1:C:274:LEU:O	2.54	0.41
1:A:84:GLN:CA	1:A:84:GLN:NE2	2.84	0.41
1:B:58:ASP:OD2	1:B:59:MET:N	2.54	0.41
1:B:371:ALA:N	1:B:426:GLY:O	2.54	0.41
1:D:341:ASP:CG	1:D:341:ASP:O	2.59	0.41
1:A:371:ALA:N	1:A:426:GLY:O	2.54	0.41
1:A:303:GLY:O	1:A:311:ARG:NE	2.54	0.40
1:A:89:LYS:NZ	1:A:221:LEU:O	2.54	0.40
1:B:299:LYS:NZ	3:B:676:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/385 (84%)	299 (93%)	24 (7%)	0	100	100
1	B	320/385 (83%)	292 (91%)	28 (9%)	0	100	100
1	C	323/385 (84%)	298 (92%)	25 (8%)	0	100	100
1	D	320/385 (83%)	296 (92%)	23 (7%)	1 (0%)	50	54
All	All	1286/1540 (84%)	1185 (92%)	100 (8%)	1 (0%)	59	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	364	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/299 (85%)	233 (92%)	20 (8%)	18	15
1	B	252/299 (84%)	222 (88%)	30 (12%)	8	5
1	C	253/299 (85%)	219 (87%)	34 (13%)	6	3
1	D	253/299 (85%)	225 (89%)	28 (11%)	9	6
All	All	1011/1196 (84%)	899 (89%)	112 (11%)	9	6

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	24	ASP
1	A	31	SER
1	A	33	LYS
1	A	74	LYS
1	A	80	GLN
1	A	83	GLU
1	A	87	LYS
1	A	216	ASP
1	A	218	GLN
1	A	230	THR

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Mol	Chain	Res	Type
1	A	250	LEU
1	A	258	GLN
1	A	280	ASN
1	A	346	TYR
1	A	370	VAL
1	A	376	GLU
1	A	453	PHE
1	A	469	LEU
1	A	470	GLU
1	B	7	VAL
1	B	26	LEU
1	B	30	VAL
1	B	76	MET
1	B	93	SER
1	B	204	ILE
1	B	217	LYS
1	B	227	VAL
1	B	234	MET
1	B	235	THR
1	B	238	ASP
1	B	251	ASP
1	B	258	GLN
1	B	260	VAL
1	B	274	LEU
1	B	287	THR
1	B	309	THR
1	B	326	ASP
1	B	345	LYS
1	B	376	GLU
1	B	380	TYR
1	B	383	ARG
1	B	384	GLN
1	B	422	VAL
1	B	431	THR
1	B	434	GLN
1	B	449	GLN
1	B	455	ARG
1	B	456	GLU
1	B	459	GLN
1	C	4	SER
1	C	5	LYS
1	C	6	PHE

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Mol	Chain	Res	Type
1	C	34	THR
1	C	53	THR
1	C	79	GLU
1	C	83	GLU
1	C	93	SER
1	C	201	ILE
1	C	205	GLU
1	C	206	LYS
1	C	212	ASN
1	C	220	ARG
1	C	230	THR
1	C	251	ASP
1	C	260	VAL
1	C	262	ASP
1	C	273	SER
1	C	285	GLU
1	C	306	SER
1	C	309	THR
1	C	344	ILE
1	C	345	LYS
1	C	362	MET
1	C	366	MET
1	C	377	THR
1	C	378	GLU
1	C	383	ARG
1	C	384	GLN
1	C	385	PHE
1	C	424	TYR
1	C	445	TYR
1	C	462	ARG
1	C	468	LEU
1	D	14	ASP
1	D	52	ASP
1	D	59	MET
1	D	65	ARG
1	D	74	LYS
1	D	85	VAL
1	D	201	ILE
1	D	202	LYS
1	D	218	GLN
1	D	230	THR
1	D	232	ASP

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Mol	Chain	Res	Type
1	D	242	LYS
1	D	251	ASP
1	D	258	GLN
1	D	260	VAL
1	D	308	CYS
1	D	309	THR
1	D	310	THR
1	D	312	VAL
1	D	316	VAL
1	D	339	ILE
1	D	341	ASP
1	D	363	LEU
1	D	370	VAL
1	D	388	TYR
1	D	453	PHE
1	D	459	GLN
1	D	464	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	501	-	3,3,3	0.45	0	2,2,2	1.03	0
2	EDO	A	502	-	3,3,3	0.40	0	2,2,2	0.50	0
2	EDO	A	503	-	3,3,3	0.53	0	2,2,2	0.11	0
2	EDO	B	501	-	3,3,3	0.54	0	2,2,2	0.38	0
2	EDO	C	501	-	3,3,3	0.34	0	2,2,2	0.65	0
2	EDO	D	501	-	3,3,3	0.37	0	2,2,2	0.82	0
2	EDO	D	502	-	3,3,3	0.45	0	2,2,2	0.31	0
2	EDO	D	503	-	3,3,3	0.40	0	2,2,2	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	501	-	-	0/1/1/1	0/0/0/0
2	EDO	A	502	-	-	0/1/1/1	0/0/0/0
2	EDO	A	503	-	-	0/1/1/1	0/0/0/0
2	EDO	B	501	-	-	0/1/1/1	0/0/0/0
2	EDO	C	501	-	-	0/1/1/1	0/0/0/0
2	EDO	D	501	-	-	0/1/1/1	0/0/0/0
2	EDO	D	502	-	-	0/1/1/1	0/0/0/0
2	EDO	D	503	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/385 (85%)	0.07	11 (3%) 43 48	24, 41, 77, 128	0
1	B	328/385 (85%)	0.03	3 (0%) 81 86	24, 43, 79, 143	0
1	C	329/385 (85%)	0.17	11 (3%) 44 50	29, 49, 91, 141	0
1	D	328/385 (85%)	0.07	9 (2%) 52 59	27, 45, 82, 161	0
All	All	1313/1540 (85%)	0.08	34 (2%) 53 60	24, 45, 84, 161	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	ILE	7.2
1	A	293	ALA	5.6
1	C	309	THR	5.4
1	C	7	VAL	5.1
1	B	379	ILE	5.0
1	A	388	TYR	4.6
1	A	255	GLY	4.6
1	C	432	VAL	4.2
1	D	461	ILE	4.0
1	A	25	VAL	3.6
1	C	6	PHE	3.5
1	D	318	VAL	3.5
1	A	243	ALA	3.2
1	C	383	ARG	3.2
1	D	301	GLY	3.1
1	D	469	LEU	3.0
1	A	256	HIS	2.7
1	C	325	TYR	2.7
1	D	317	GLY	2.7
1	A	251	ASP	2.6
1	B	344	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	0	ALA	2.5
1	C	429	ALA	2.5
1	A	470	GLU	2.5
1	C	367	PHE	2.5
1	C	208	ILE	2.3
1	A	26	LEU	2.3
1	B	380	TYR	2.3
1	D	208	ILE	2.3
1	A	347	SER	2.2
1	D	315	GLY	2.2
1	C	229	VAL	2.2
1	A	204	ILE	2.1
1	D	207	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	B	501	4/4	0.18	6.31	82,83,87,89	0
2	EDO	D	503	4/4	0.13	1.13	38,39,40,40	0
2	EDO	A	501	4/4	0.11	-0.62	40,41,43,46	0
2	EDO	C	501	4/4	0.10	-1.16	41,42,43,45	0
2	EDO	D	502	4/4	0.10	-2.83	35,36,41,42	0
2	EDO	A	503	4/4	0.12	-	44,47,48,52	0
2	EDO	A	502	4/4	0.12	-	57,60,63,65	0
2	EDO	D	501	4/4	0.15	-	39,45,47,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.